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INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

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INCODELED ANDIBAD.

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98.3% PROCESSED 834112 ITERATIONS

19 ANSWERS

100.0% PROCESSED 848347 ITERATIONS

19 ANSWERS

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FILE COVERS 1907 - 31 May 2006 VOL 144 ISS 23 FILE LAST UPDATED: 30 May 2006 (20060530/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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L4 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Jana Text References

ACCESSION NUMBER: 2005:140666 HCAPLUS

DOCUMENT NUMBER: 142:210949

TITLE: Artificial receptors, building blocks, and methods

INVENTOR(S): Carlson, Robert E. PATENT ASSIGNEE(S): Receptors Llc, USA

SOURCE: U.S. Pat. Appl. Publ., 72 pp., Cont.-in-part of Appl.

No. PCT/US03/05328.

CODEN: USXXCO

DOCUMENT TYPE:

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT: 14

PATENT INFORMATION:

PATENT NO.			KIND DATE				APPLICATION NO.							DATE			
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AB The present invention relates to artificial receptors and arrays or microarrays of artificial receptors or candidate artificial receptors.

Each member of the array includes a plurality of building block compds., which can be immobilized in a spot on a support. The present invention also includes the building blocks, combinations of building blocks, arrays of building blocks, and receptors constructed of these building blocks

together with a support. The present invention also includes methods of making and using these arrays and receptors.

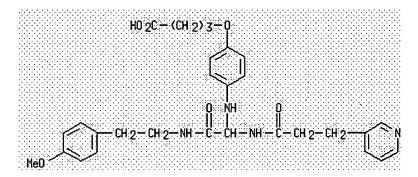
# IT 596118-78-4P

RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)

(methods for combinatorial synthesis and use of artificial receptors and building blocks)

RN 596118-78-4 HCAPLUS

Butanoic acid, 4-[4-[2-(4-methoxyphenyl)ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl)ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl)ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl)ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl)ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl)ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl)ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl)ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl)ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl)ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl)ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl)ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl)ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl)ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl)ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl]ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl]ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl]ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl]ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl]ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl]ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl]ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl]ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl]ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl]ethyl]amino]-2-oxo-1-[[1-oxo-methoxyphenyl]ethyl]amino[[1-oxo-methoxyphenyl]ethyl]amino[[1-oxo-methoxyphenyl]ethyl]amino[[1-oxo-methoxyphenyl]ethyl]amino[[1-oxo-methoxyphenyl]ethyl]amino[[1-oxo-methoxyphenyl]ethyl]amino[[1-oxo-methoxyphenyl]ethyl]amino[[1-oxo-methoxyphenyl]ethyl]amino[[1-oxo-methoxyphenyl]ethyl]amino[[1-oxo-methoxyphenyl]ethyl]amino[[1-oxo-methoxyphenyl]ethyl]amino[[1-oxo-methoxyphenyl]ethyl]amino[[1-oxo-methoxyphenyl]ethyl]amino[[1-oxo-methoxyphenyl]ethyl]amino[[1-oxo-methoxyphenyl]ethylamino[[1-oxo-methoxyphenyl]ethylamino[[1-oxo-methoxyphenyl]ethylamino[[1-oxo-methoxyphenyl]ethylamino[[1-oxo-methoxyphenyl]ethylamino[[1-oxo-methoxyphenyl]ethylamino[[1-oxo-methoxyphenyl]ethylamino[[1-oxo-methoxyphenyl]ethylamino[[1-oxo-methoxyphenyl]ethylamino[[1-oxo-methoxyphenyl]ethylamino[[1-oxo-methoxyphenyl]ethylamino[[1-oxo-methoxyphenyl]ethylamino[[1-oxo-methoxyphenyl]ethylamino[[1-oxo-methoxyphenyl]ethylamino[[1-oxo-methoxyphenyl]ethylamino[[1-oxo-mCN 3-(3-pyridinyl)propyl]amino]ethyl]amino]phenoxy]- (9CI) (CA INDEX NAME)



L4ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text References

2003:719694 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 139:254455

TITLE: Artificial receptors, building blocks, and methods

INVENTOR(S): Carlson, Robert E. PATENT ASSIGNEE(S): Receptors LLC, USA SOURCE: PCT Int. Appl., 145 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent English LANGUAGE:

FAMILY ACC. NUM. COUNT: 14

PATENT INFORMATION:

PATENT NO.	KIN	D DATE	APPLICATION NO.	DATE		
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OTHER SOURCE(S): MARPAT 139:254455

The present invention relates to artificial receptors and arrays or microarrays of artificial receptors or candidate artificial receptors. Each member of the array includes a plurality of building block compds., typically immobilized in a spot on a support. The present invention also includes the building blocks, combinations of building blocks, arrays of building blocks, and receptors constructed of these building blocks together with a support. The present invention also includes methods of making and using these arrays and receptors.

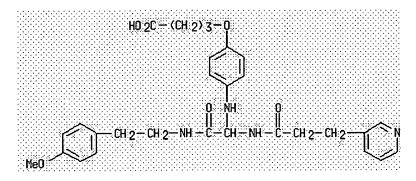
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RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)

(methods for combinatorial synthesis and use of artificial receptors and building blocks)

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CN Butanoic acid, 4-[4-[[2-[[2-(4-methoxyphenyl)ethyl]amino]-2-oxo-1-[[1-oxo-3-(3-pyridinyl)propyl]amino]ethyl]amino]phenoxy]- (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

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SSION NUMBER: 2002:256223 HCAPLUS

DOCUMENT NUMBER: 136:295089

TITLE: Preparation of amino acid aromatic derivatives with

HIV integrase inhibitory properties

INVENTOR(S): N'zemba, Blaise Magloire; Sauve, Gilles; Sevigny, Guy;

Yelle, Jocelyn

PATENT ASSIGNEE(S): Pharmacor, Inc., Can.

SOURCE: PCT Int. Appl., 173 pp.

CODEN: PIXXD2

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AU	2001	0953	10		<b>A</b> 5		2002	0408		AU 2	001-	<u>9531</u>		20010925				
US	6528	655 .			В1	1 20030304				US 2	001-	9633		20010926				
PRIORIT	Y APP	LN.	INFO	.:						CA 2000-2321348					A 20000927			
-										WO 2	001-	CA13	<u>67</u>	1	w 2	0010	925	

OTHER SOURCE(S): MARPAT 136:295089

AB Amino acid derivs. R1CO-A-CONHR2 [A = NR3CR4R5, where R3, R4 = H or Me; R5 = H, alkyl, carboxyalkyl, benzyl, MeSCH2CH2, 1-indolylmethyl, 3,4-(HO)2C6H2CH2, etc.; R3R4 may be trimethylene, which may be substituted; R1, R2 are certain rings (Ph, 3-pyridyl, 2-quinolyl, 2-thienyl, etc.), which may be substituted and attached to alkyl; R2 may also be aroylamino] were prepd. as inhibitors of HIV integrase. Thus, N-[Nα-(3,4-dihydroxybenzoyl)-Nτ-trityl-L-histidinyl]dopamine was prepd. by coupling of Nα-(9-fluorenylmethoxycarbonyl)-Nτ-trityl-

L-histidine with dopamine hydrochloride, deprotection, and acylation with 3,4-dihydroxybenzoic acid and showed anti-integrase activity IC50 = 65 nM.

# IT 406727-71-7P 406727-72-8P

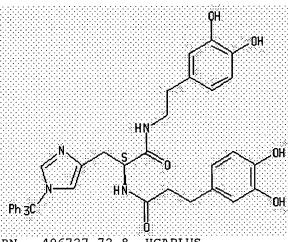
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(prepn. of amino acid arom. derivs. with HIV integrase inhibitory properties)

RN 406727-71-7 HCAPLUS

CN 1H-Imidazole-4-propanamide, N-[2-(3,4-dihydroxyphenyl)ethyl]- $\alpha$ -[[3-(3,4-dihydroxyphenyl)-1-oxopropyl]amino]-1-(triphenylmethyl)-, (αS)-(CA INDEX NAME)

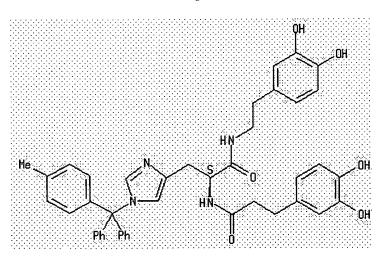
Absolute stereochemistry.



406727-72-8 HCAPLUS RN

1H-Imidazole-4-propanamide, N-[2-(3,4-dihydroxyphenyl)ethyl]- $\alpha$ -[[3-CN (3, 4-dihydroxyphenyl)-1-oxopropyl]amino]-1-[(4methylphenyl)diphenylmethyl]-, (\alpha S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



HCAPLUS COPYRIGHT 2006 ACS on STN L4ANSWER 4 OF 7

Text ACCESSION NUMBER:

DOCUMENT NUMBER:

2002:237355 HCAPLUS

136:263476

TITLE:

Preparation of hydroxyphenyl derivatives with HIV

integrase inhibitory properties

INVENTOR (S):

Sauve, Gilles; Yelle, Jocelyn

PATENT ASSIGNEE(S):

Pharmacor Inc., Can.

SOURCE:

U.S., 36 pp., Cont.-in-part of U.S. Ser. No. 280,569,

abandoned.

CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

anti-integrase activity IC50 = 100  $\mu$ M.

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>US 6362165</u>	В1	20020326	<u>US 2000-534615</u>	20000327
PRIORITY APPLN. INFO.:			<u>US 1999-280569</u> B2	19990330
OTHER SOURCE(S):	MARPAT	136:263476		

Amino acid hydroxyphenyl derivs. 3,4-(HO)2C6H3-X-NH-W-CO-X'-R and [3,4-(HO)2C6H3CH2CH2NHCOCH(NRaCOR)CH2S]2 [R is Ph substituted by 1-3 OH groups and 0-2 halo group; X, X' = a single bond, C1-4 alkylene or C2-4 alkenylene; Ra = H, Me; W = -A-CO(A'CO)n-, where n = 0 or 1 and A, A' are -NRaCRbRc- (Ra, Rb = H, Me; Rc = H, Me, Me2CH, PHCH2, HO2CCH2, 3-indolylmethyl, 3-guanidylpropyl, 3,4-dihydroxybenzyl, etc. or RaRc together form an azole ring which may be substituted by hydroxy) (with provisos)] were prepd. as inhibitors of HIV integrase. Thus, N-[N-(3,4-dihydroxybenzoyl)glycyl]dopamine, prepd. from glycine tert-Bu ester via coupling with 3,4-dihydroxybenzoic acid and dopamine, showed

# IT 300409-28-3P

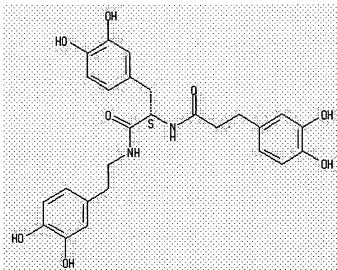
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of amino acid hydroxyphenyl derivs. with HIV integrase inhibitory properties)

RN 300409-28-3 HCAPLUS

CN Benzenepropanamide, N-[2-(3,4-dihydroxyphenyl)ethyl]- $\alpha$ -[[3-(3,4-dihydroxyphenyl)ethyl]- $\alpha$ -[3-(3,4-dihydroxyphenyl)ethyl]- $\alpha$ -[3-(3,4-dihydroxyphenyl)eth dihydroxyphenyl)-1-oxopropyl]amino]-3,4-dihydroxy-,  $(\alpha S)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



55

REFERENCE COUNT:

THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN
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FUI) References Text

ACCESSION NUMBER:

2000:725598 HCAPLUS

DOCUMENT NUMBER:

133:282085

TITLE:

Preparation of hydroxyphenyl derivatives with HIV

integrase inhibitory properties

INVENTOR(S):

Sauve, Gilles; Yelle, Jocelyn

PATENT ASSIGNEE(S): SOURCE:

Pharmacor Inc., Can. PCT Int. Appl., 122 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.						KIND DATE			APPL:	ICAT:	I NO	DATE				
	2000				A1	-	2000	1012	]	WO 2	000-0	CA32	 <u>7</u>		2	0000	327
	w:	ΑE,	AL,	AM,	AT,	ΑU,	ΑZ,	BA,	BB,	ВG,	BR,	BY,	CH,	CN,	CR,	CU,	CZ,
		DE,	DK,	DM,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	ΗU,	ID,	IL,	IN,
		IS,	JP,	KE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,
		MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,
		SL,	ТJ,	TM,	TR,	TT,	TZ,	UA,	UG,	UŻ,	VN,	YU,	ZA,	ZW,	AM,	ΑZ,	BY,
		ΚG,	ΚZ,	MD,	RU,	ТJ,	TM										
	RW:	GH,	GM,	ΚE,	LS,	MW,	SD,	SL,	SZ,	TZ,	UG,	ZW,	ΑT,	BE,	CH,	CY,	DE,
		DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,
		CG,	CI,	CM,	GΑ,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG				
CA	2267	657			AA 20000930					CA 1	999-	<u> 2267</u>	19990330				
CA	2302	144			AA 20000930				CA 2	000-	2302	20000327					
EP	1165	492			A1		2002	0102		EP 2	000-	9139	80		2	0000	327
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GΒ,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		ΙE,	SI,	LT,	LV,	FI,	RO										
PRIORIT	Y APP	LN.	INFO	.:						CA 1	999-	<u> 2267</u>	<u>657</u>		A 1	9990	330
										US 1	999-	2805	<u>69</u>		A 1	9990	330
										WO 2	000-	CA32	<u>7</u>	•	₩ 2	0000	327

MARPAT 133:282085 OTHER SOURCE(S):

Amino acid hydroxyphenyl derivs. 3,4-(HO)2C6H3-X-NH-W-CO-X'-R and [3,4-(HO)2C6H3CH2CH2NHCOCH(NRaCOR)CH2S]2 [R is Ph substituted by 1-3 OH groups and 0-2 halo group; X, X' = a single bond, C1-4 alkylene or C2-4 alkenylene; Ra = H, Me; W = -A-CO(A'CO)n-, where n = 0 or 1 and A, A' are -NRaCRbRc- (Ra, Rb = H, Me; Rc = H, Me, Me2CH, PHCH2, HO2CCH2, benzyloxycarbonyl, 3-indolylmethyl, 3-guanidylpropyl, 3,4-dihydroxybenzyl, etc. or RaRc together form an azole ring which may be substituted by hydroxy), -NRaCRbRcCH2-, -NRaCRbRcCH2CH2] were prepd. as inhibitors of HIV integrase. Thus, N-[N-(3,4-hydroxybenzoyl)glycyl]dopamine, prepd. from glycine tert-Bu ester via coupling with 3,4-dihydroxybenzoic acid and dopamine, showed anti-integrase activity IC50 = 100 μM.

#### IT 300409-28-3P

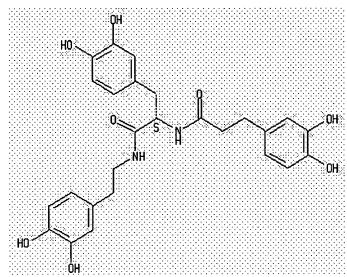
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of hydroxyphenyl derivs. with HIV integrase inhibitory properties)

RN 300409-28-3 HCAPLUS

Benzenepropanamide, N-[2-(3,4-dihydroxyphenyl)ethyl]- $\alpha$ -[[3-(3,4-CN dihydroxyphenyl)-1-oxopropyl]amino]-3,4-dihydroxy-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

# Absolute stereochemistry.



REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Milital Text References

ACCESSION NUMBER: 1998:661011 HCAPLUS

DOCUMENT NUMBER: 130:76286

TITLE: NPY Y1 antagonists: structure-activity relationships

of arginine derivatives and hybrid compounds with

arpromidine-like partial structures

AUTHOR(S): Aiglstorfer, Iris; Uffrecht, Anka; Gessele, Karin;

Moser, Christiane; Schuster, Andreas; Merz, Stefanie; Malawska, Barbara; Bernhardt, Gunther; Dove, Stefan;

Buschauer, Armin

CORPORATE SOURCE: Institute of Pharmacy, University of Regensburg,

Regensburg, D-93040, Germany

SOURCE: Regulatory Peptides (1998), 75-76, 9-21

CODEN: REPPDY; ISSN: 0167-0115

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

Previously,  $\omega$ -guanidino- and  $\omega$ -aminoalkanamides, structurally derived from arpromidine-like histamine H2 receptor agonists, were reported as novel neuropeptide Y Y1 antagonists. Regardless of the backbone, they resemble BIBP 3226, an argininamide with high NPY Y1 receptor affinity and selectivity, with respect to nature and arrangement of the 'terminal' diaryl, guanidine, and hydroxyphenyl groups. Hybrid compds. were synthesized combining the argininamide backbone of BIBP 3226 or partial structures derived from the C-terminal dipeptide of NPY with characteristic substructures of arpromidine- or amide-type NPY antagonists. Addnl., some analogs of BIBP 3226 with reduced flexibility were prepd. Structure-activity relationships indicate that, in contrast to alkanamides, homologs and/or isomers of BIBP 3226 with vicinal arrangement of the Ph rings have decreased Y1 antagonistic activity (Ca2+-assay in HEL cells). Replacement of the hydroxybenzyl group by an imidazole ring further decreases activity. It is concluded that the binding sites of NPY antagonists with one and with two basic groups are not identical. Analogs with a rigid tetrahydro-2-benzazepine or an indan group in place of the benzyl moiety in BIBP 3226 are active, indicating the role of the OH group and supporting the model proposed for the interaction of BIBP 3226 with the Y1 receptor.

# IT <u>218793-28-3</u>P <u>218793-31-8</u>P <u>218793-45-4</u>P

# 218793-47-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; neuropeptide Y Y1 receptor antagonists and structure-activity relationships of arginine derivs. and hybrid compds. with arpromidine-like partial structures)

RN 218793-28-3 HCAPLUS

CN 2H-Isoindole-2-pentanamide,  $\alpha$ -[[4-(3,4-dichlorophenyl)-1-oxo-4-(2-pyridinyl)butyl]amino]-1,3-dihydro-N-[2-(4-methoxyphenyl)ethyl]-1,3-dioxo-, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN <u>218793-31-8</u> HCAPLUS

CN

2-Pyridinebutanamide, N-[(1S)-4-amino-1-[[[2-(4-methoxyphenyl)ethyl]amino]carbonyl]butyl]-γ-(3,4-dichlorophenyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 218793-45-4 HCAPLUS

CN Benzenepropanamide, N-[(1S)-1-[[[2-(4-hydroxyphenyl)ethyl]amino]carbonyl]-4-[[imino(nitroamino)methyl]amino]butyl]- $\beta$ -phenyl- (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

RN 218793-47-6 HCAPLUS

CN Benzenepropanamide, N-[(1R)-1-[[[2-(4-hydroxyphenyl)ethyl]amino]carbonyl]-4-[[imino(nitroamino)methyl]amino]butyl]- $\beta$ -phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 218792-94-0P 218792-97-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(neuropeptide Y Y1 receptor antagonists and structure-activity relationships of arginine derivs. and hybrid compds. with arpromidine-like partial structures)

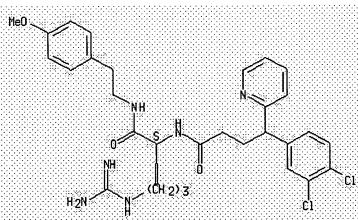
RN 218792-94-0 HCAPLUS

CN

CN

2-Pyridinebutanamide, N-[(1S)-4-[(aminoiminomethyl)amino]-1-[[[2-(4-methoxyphenyl)ethyl]amino]carbonyl]butyl]- $\gamma$ -(3,4-dichlorophenyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 218792-97-3 HCAPLUS

Benzenepropanamide, N-[4-[(aminoiminomethyl)amino]-1-[[[2-(4-hydroxyphenyl)ethyl]amino]carbonyl]butyl]- $\beta$ -phenyl- (9CI) (CA INDEX

NAME)

O NH - C - CH<sub>2</sub>- CHPh<sub>2</sub>
CH<sub>2</sub>- CH<sub>2</sub>- CH - C- CH - (CH<sub>2</sub>)<sub>3</sub>-NH - C-NH<sub>2</sub>
NH

REFERENCE COUNT:

THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

25

Full Cities Text Relevence:

ACCESSION NUMBER: 1995:620466 HCAPLUS

DOCUMENT NUMBER: 123:257350

TITLE: Trifunctional reagents for derivatizing sulfhydryl

groups

AUTHOR(S): Finn, Frances M.; Yamanouchi, Keitaro; Titus, Gail;

Hofmann, Klaus

CORPORATE SOURCE: Dep. Med., Univ. Pittsburgh, Pittsburgh, PA, 15261,

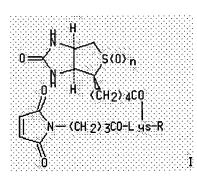
USA

SOURCE: Bioorganic Chemistry (1995), 23(2), 152-68

CODEN: BOCMBM; ISSN: 0045-2068

PUBLISHER: Academic
DOCUMENT TYPE: Journal
LANGUAGE: English

GΙ



The syntheses of four trifunctional reagents I (n = 0, 2, R =AB NHCH2CH2C6H4OH-4; n = 0, R = Tyr-OH, NHCH2CH2NHCOCH2CH2C6H4OH-4) for alkylating sulfhydryl groups in proteins are described. Each reagent I contains a maleimide function capable of reacting with SH groups, a p-hydroxyphenyl group that can be iodinated, and a "biotin handle" to facilitate purifn. of the derivatized proteins or peptides derived from them by biotin-avidin affinity chromatog. Detailed conditions for obtaining the pure diiodo derivs. of I have been developed. The biotin is attached to all the reagents via the  $\epsilon$ -amino group of lysine (biocytin) to provide sufficient space for optimum binding to avidin. half-times (t1/2) for dissocn. of I (n = 0, R = CH2CH2C6H4OH-4) from succinoyl avidin (36.7 days), monoiodo (26.1 days) and diiodo derivs. (21.4 days), and sulfone I (n = 2, R = NHCH2CH2C6H4OH-4) (29.8 days), demonstrate that iodination does not significantly interfere with binding of the biotin residue to succinoyl avidin and that these reagents can be used effectively as affinity ligands. Remarkably, all the reagents I can

be iodinated without loss of the sulfhydryl alkylating capacity. Alkylation of highly purified human placental insulin receptor with the di-iodo derivs. of the reagents results in significant incorporation of 125I into the b-subunit of the receptor and the alkylation was prevented by prior exposure of the receptor to NEM. The advantages of these reagents over those previously available are that the parent mols. (1) are inexpensive to prep., (2) are solids that can be stored indefinitely without degrdn., (3) and can be radiolabeled to specific activity levels over seventy times higher with 125I than the specific activity available for 3H derivs.

# IT 168639-58-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (prepn. of trifunctional reagents for derivatizing protein sulfhydryl groups)

RN 168639-58-5 HCAPLUS

CN 1H-Thieno[3,4-d]imidazole-4-pentanamide, N-[5-[[4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxobutyl]amino]-6-[[2-(4-hydroxyphenyl)ethyl]amino]-6- oxohexyl]hexahydro-2-oxo-, [3aS-[3aα,4β(R\*),6aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

# IT 168639-67-6P 168639-81-4P 168639-82-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. of trifunctional reagents for derivatizing protein sulfhydryl groups)

RN <u>168639-67-6</u> HCAPLUS

CN

1H-Thieno[3,4-d]imidazole-4-pentanamide, N-[5-[[4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxobutyl]amino]-6-[[2-(4-hydroxyphenyl)ethyl]amino]-6-oxohexyl]hexahydro-2-oxo-, 5,5-dioxide, [3aS-[3a $\alpha$ ,4 $\beta$ (R\*),6a.alpha.]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 168639-81-4 HCAPLUS

TH-Thieno[3, 4-d]imidazole-4-pentanamide, N-[5-[[4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxobutyl]amino]-6-[[2-(4-hydroxy-3-iodophenyl)ethyl]amino]-6-oxohexyl]hexahydro-2-oxo-, [3aS-[3aα, 4β(R\*), 6aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 168639-82-5 HCAPLUS

CN 1H-Thieno[3,4-d]imidazole-4-pentanamide, N-[5-[[4-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)-1-oxobutyl]amino]-6-[[2-(4-hydroxy-3,5-diiodophenyl)ethyl]amino]-6-oxohexyl]hexahydro-2-oxo-,
[3aS-[3aα,4β(R\*),6aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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